Temperature-induced boomerang/revolving effect of electron flow in semiconductor heterostructures

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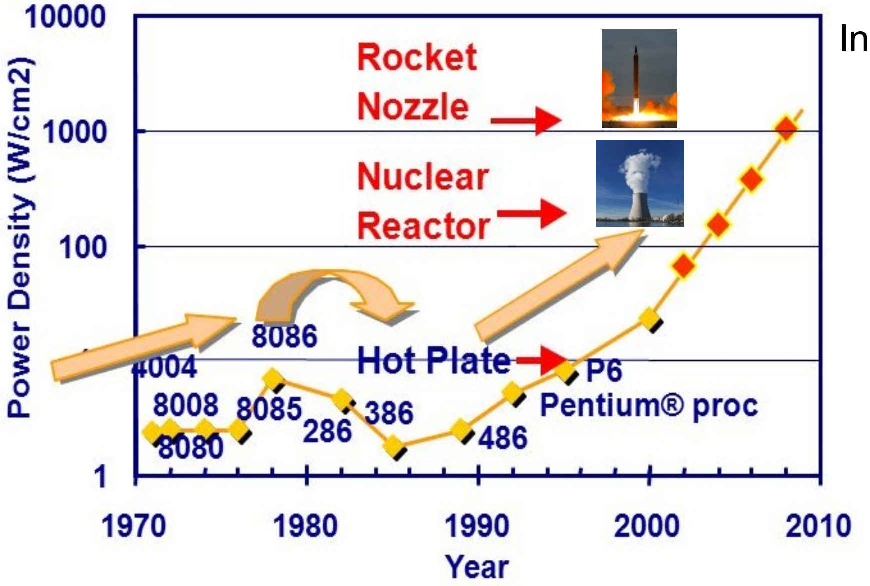
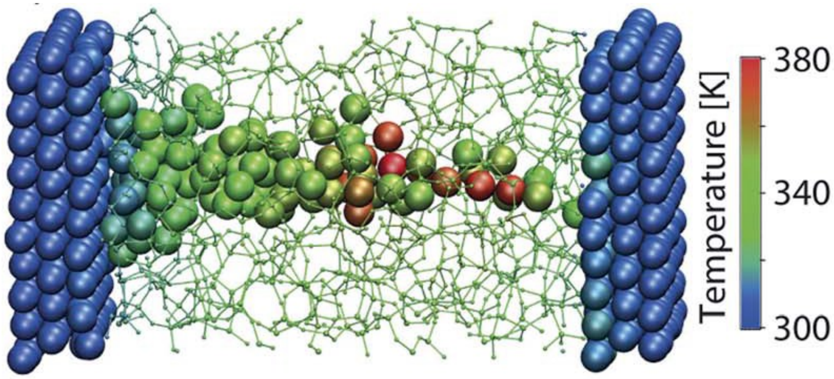
Cooling at the nanoscale

- **Self-heating: scientific and industrial issues**



Intel, 2004



CBRAM

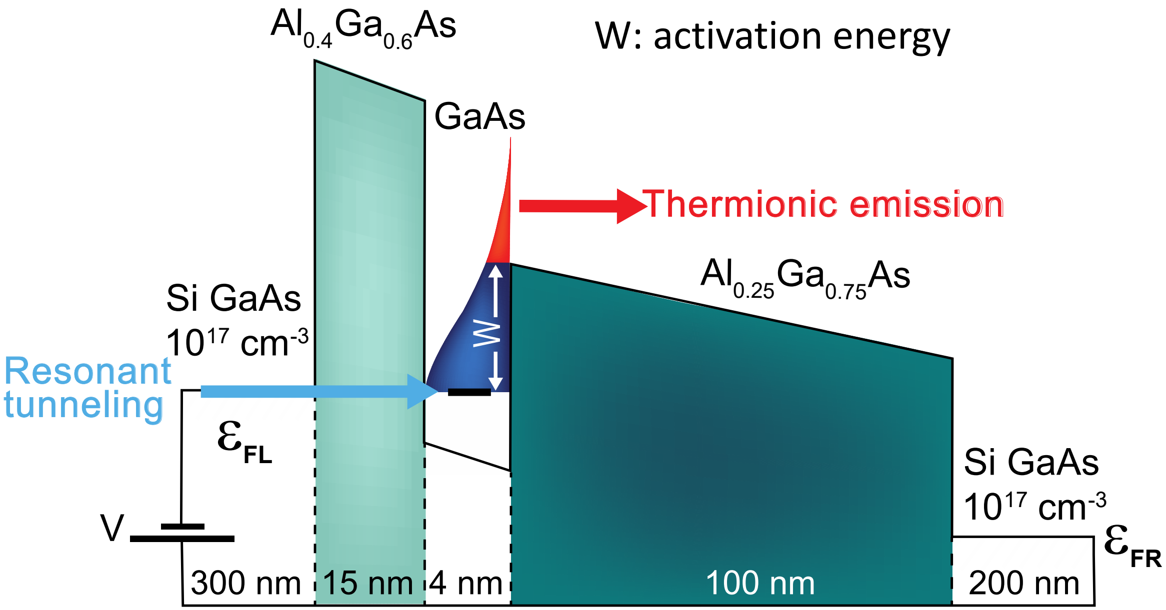
Nanoscale Adv., **2,** 2648 (2020)
M. Luisier, ETH Zurich

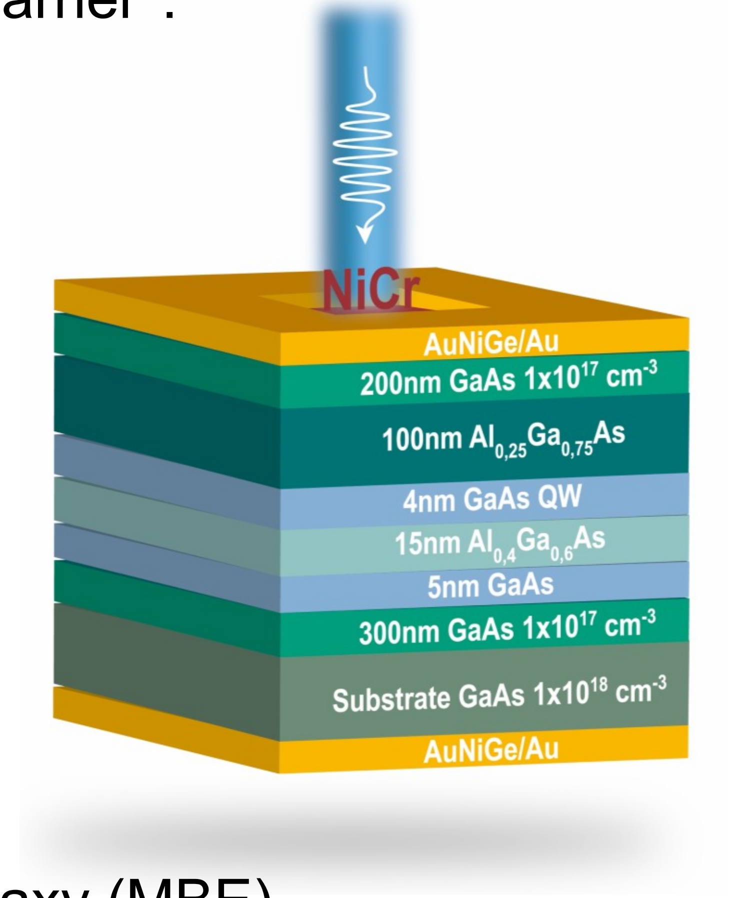
- Significant reduction of lifetimes and performances.
- “Bulk” refrigeration is extremely power consuming.

Urgent need of local source of cooling

Experimental implementation

- ➢ Coupling localized state and tunneling barrier*:

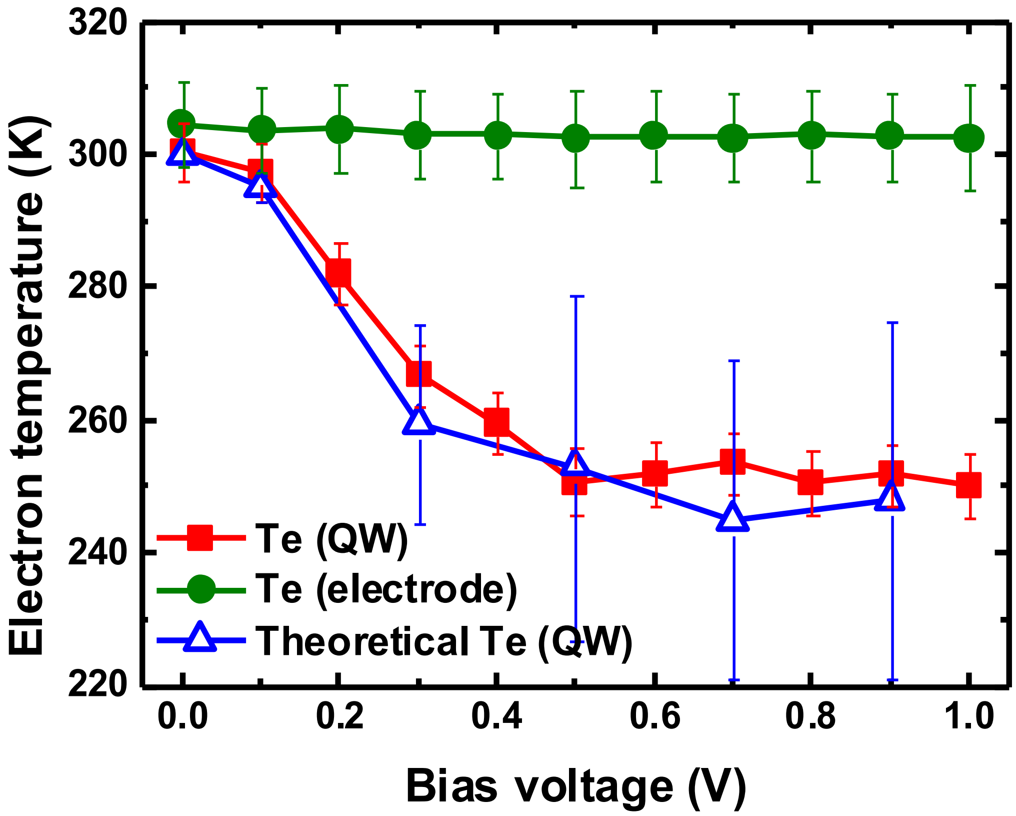


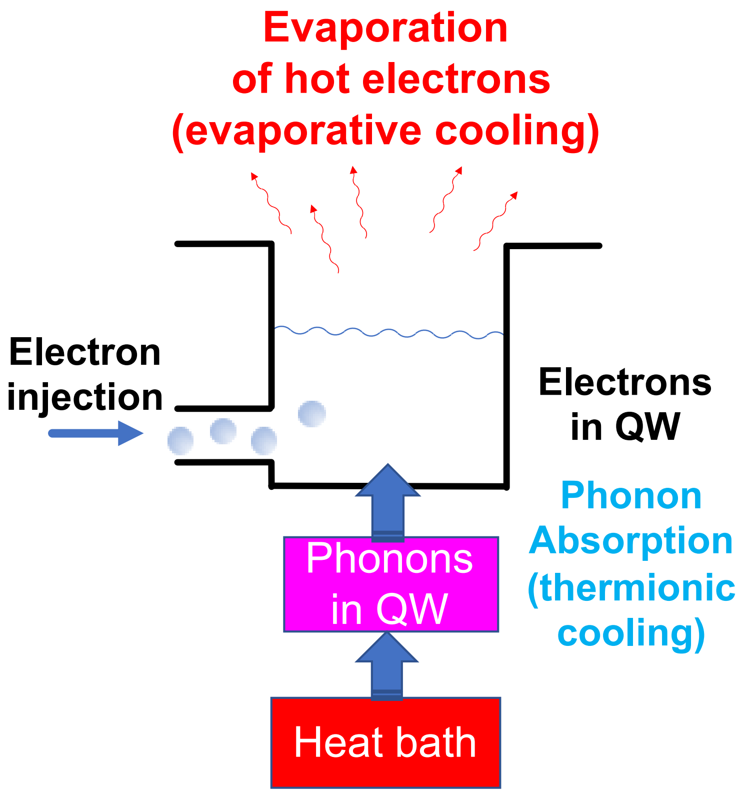


- ➢ Sample fabrication: Molecular beam epitaxy (MBE).
- ➢ Temperature of electron T_e in the quantum well (QW).

*A. Yangui, M. Bescond, T. Yan, N. Nagai, and K. Hirakawa, *Nature Commun*. **10**, 4504 (2019).

Electron Temperature(s)*





Evaporation of hot electrons (evaporative cooling)

Electron injection

Electrons in QW

Phonon Absorption (thermionic cooling)

Phonons in QW

Heat bath

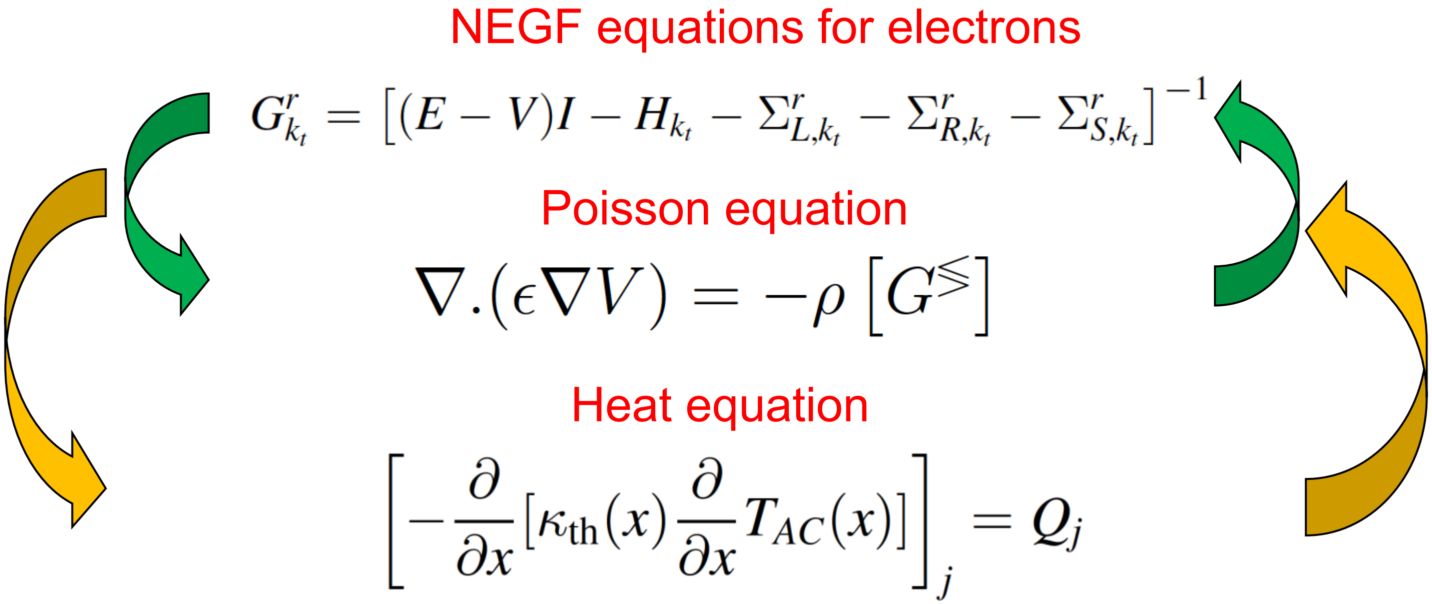
- ➢ T_e in electrodes constant.
- ➢ T_e in the QW decreases by 50K due to evaporative cooling.

*A. Yangui, M. Bescond, T. Yan, N. Nagai, and K. Hirakawa, *Nature Commun*. **10**, 4504 (2019).

*M. Bescond, *et al.*, *Phys. Rev. Appl.* **17,** 014001 (2022).

NEGF + Heat equation

- **Non-equilibrium Green's function coupled to heat equation***



NEGF equations for electrons

$$G^r_{k_t} = \left[(E - V)I - H_{k_t} - \Sigma^r_{L,k_t} - \Sigma^r_{R,k_t} - \Sigma^r_{S,k_t}\right]^{-1}$$

Poisson equation

$$\nabla.(\epsilon\nabla V) = -\rho\left[G^{\lessgtr}\right]$$

Heat equation

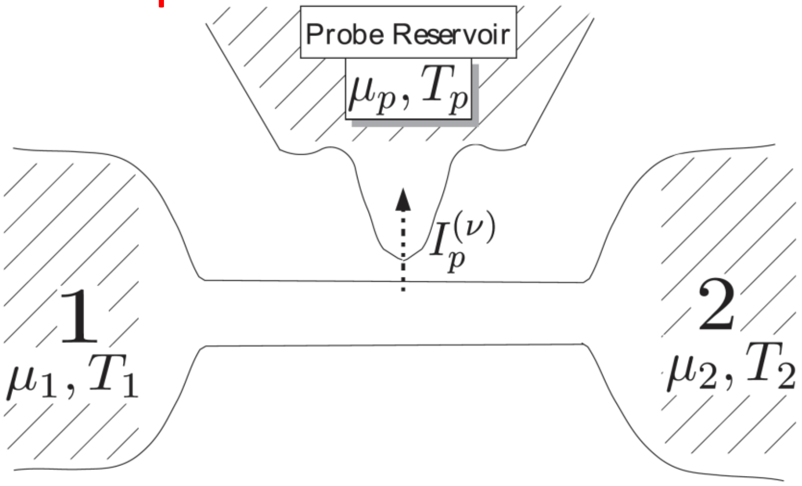
$$\left[-\frac{\partial}{\partial x}\left[\kappa_{\text{th}}(x)\frac{\partial}{\partial x}T_{AC}(x)\right]\right]_j = Q_j$$

- Most of physical properties: current, electron density, LDOS, local phonon temperatures, cooling power, efficiency…
- But… We are in a strong non-equilibrium regime… $T_{AC} \neq T_{POP} \neq T_e$
- Temperature of electrons in the active region???

Electronic temperature: virtual probe technique

- System out of equilibrium:
  Electronic and lattice temperatures usually not coincide.
- Accurate electronic temperature measurement (i.e. that follows the thermodynamic laws) requires simultaneously local voltage measurement.[1,2]
- Technique: vanish net charge current ($I_p^{(0)}$) **and** net heat current ($I_p^{(1)}$) into the probe.
  --> probe in local equilibrium with the sample.

$$I_p^{(\nu)} = 0, \quad \nu \in \{0, 1\}$$



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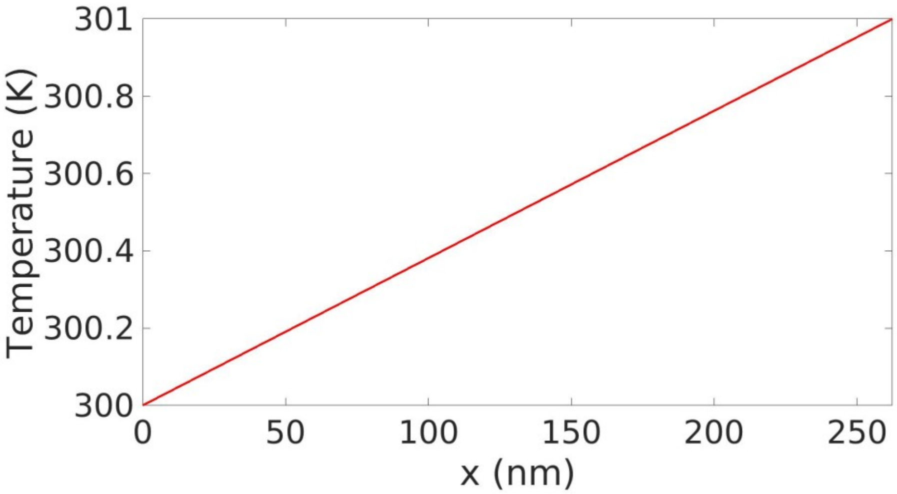
[1] C. A. Stafford, *Phys. Rev. B* **93**, 245403 (2016).

[2] A. Shastry and C. A. Stafford, *Phys. Rev. B* **94**, 155433 (2016).

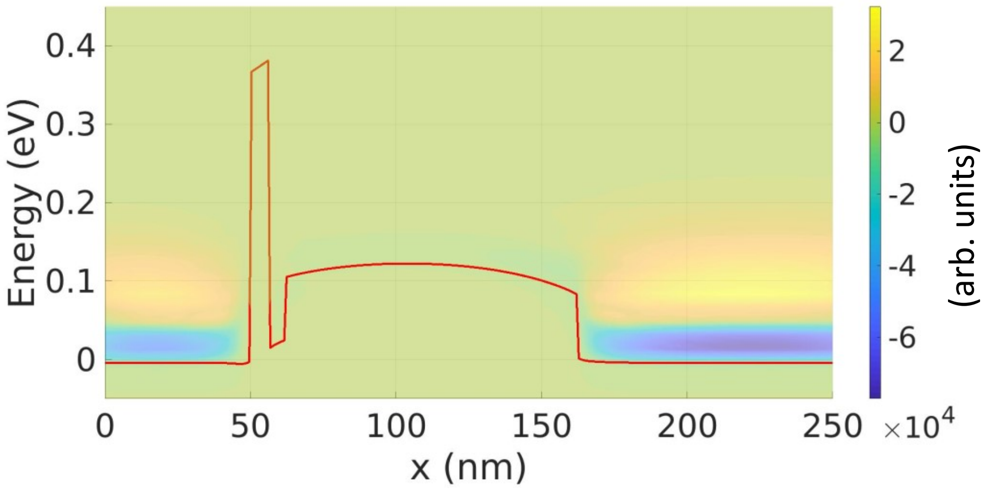
Response to a temperature gradient

Lattice temperature gradient

ΔT=1 K



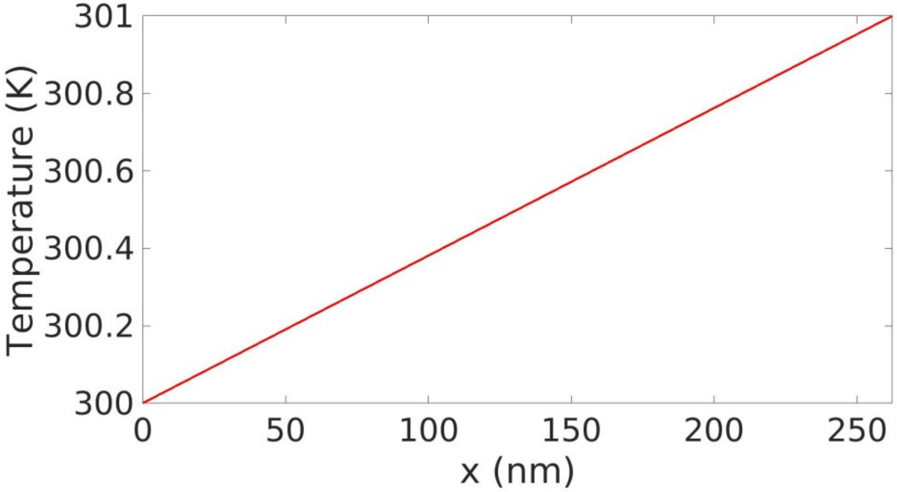
Current spectrum



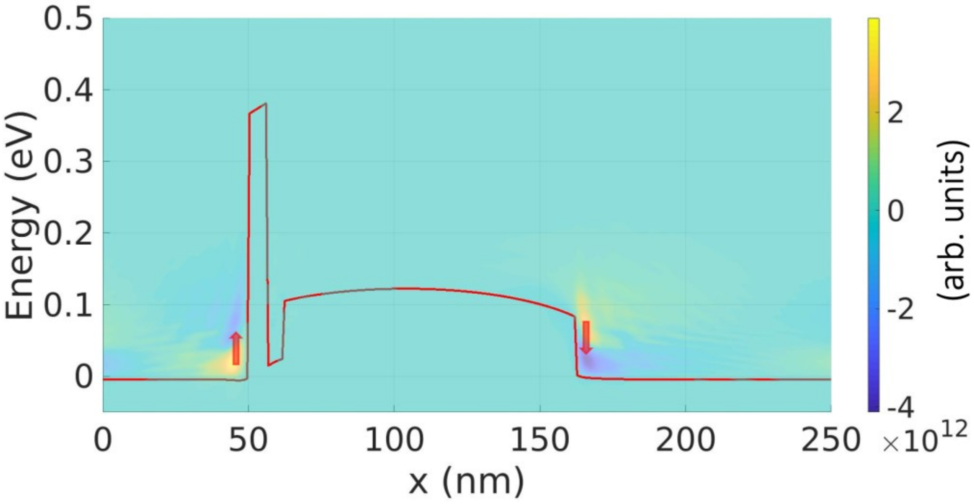
- ➢ Two current components in the access regions.
- ➢ At the barrier: phonon emission/absorption and back flow towards the contacts

Lattice temperature gradient

ΔT=1 K



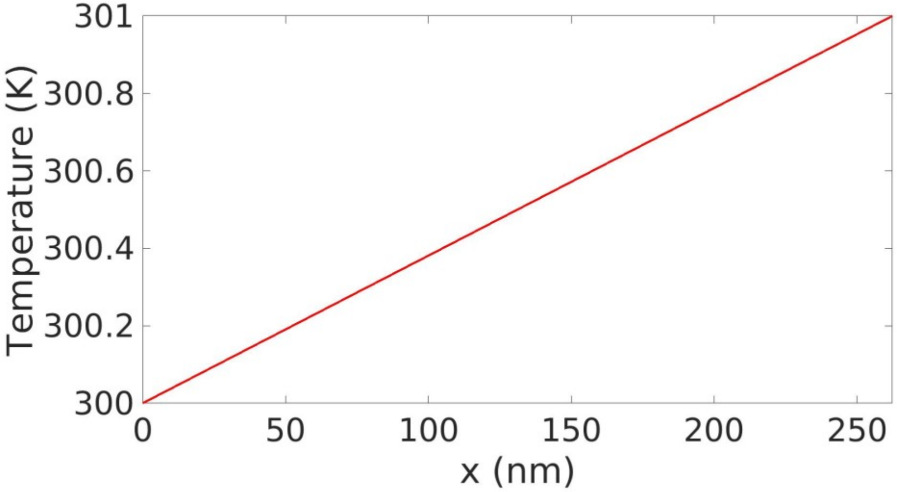
Derivative of energy current



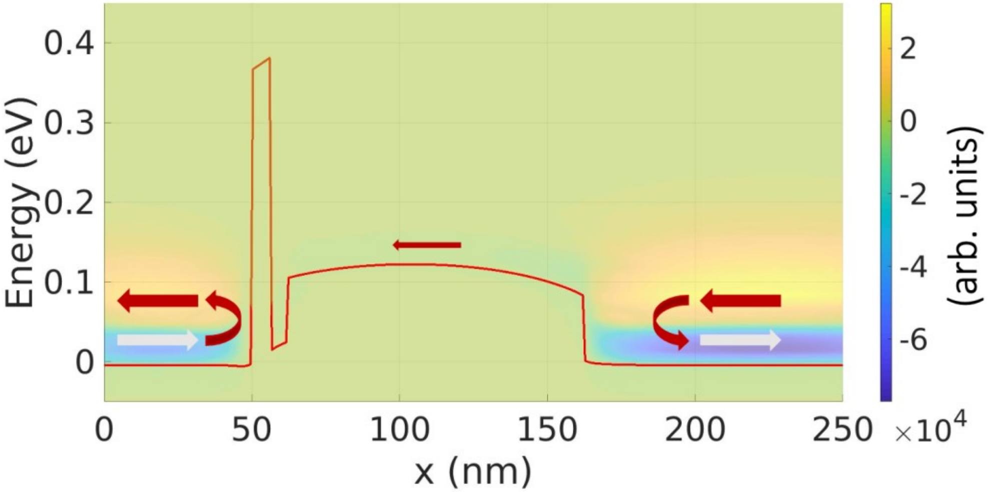
- ➢ Two current components in the access regions.
- ➢ At the barrier: phonon emission/absorption and back flow towards the contacts

Lattice temperature gradient

ΔT=1 K



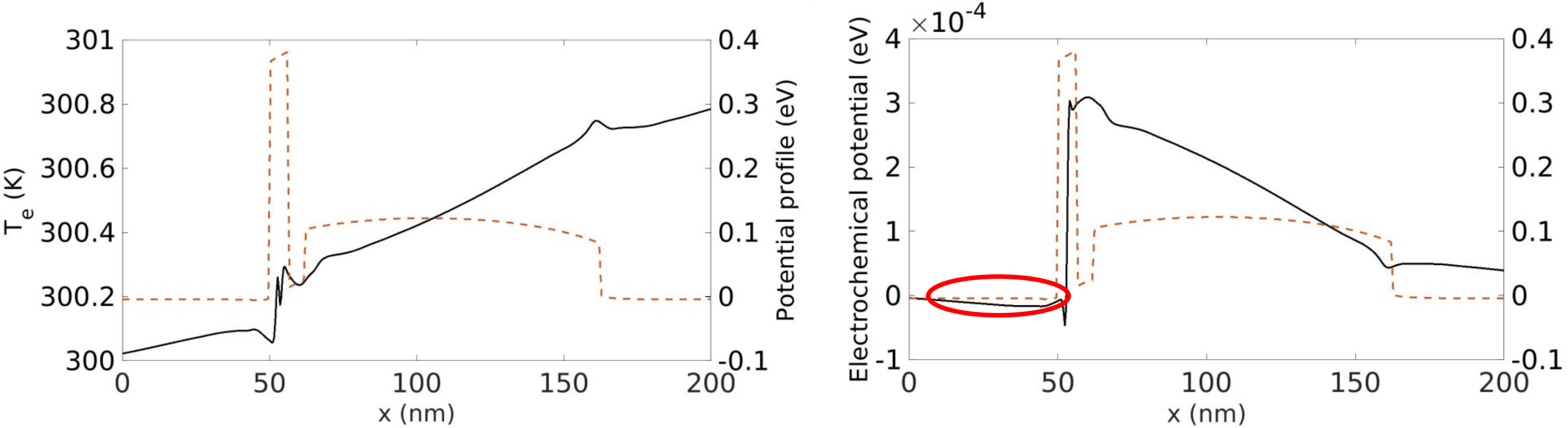
Current spectrum



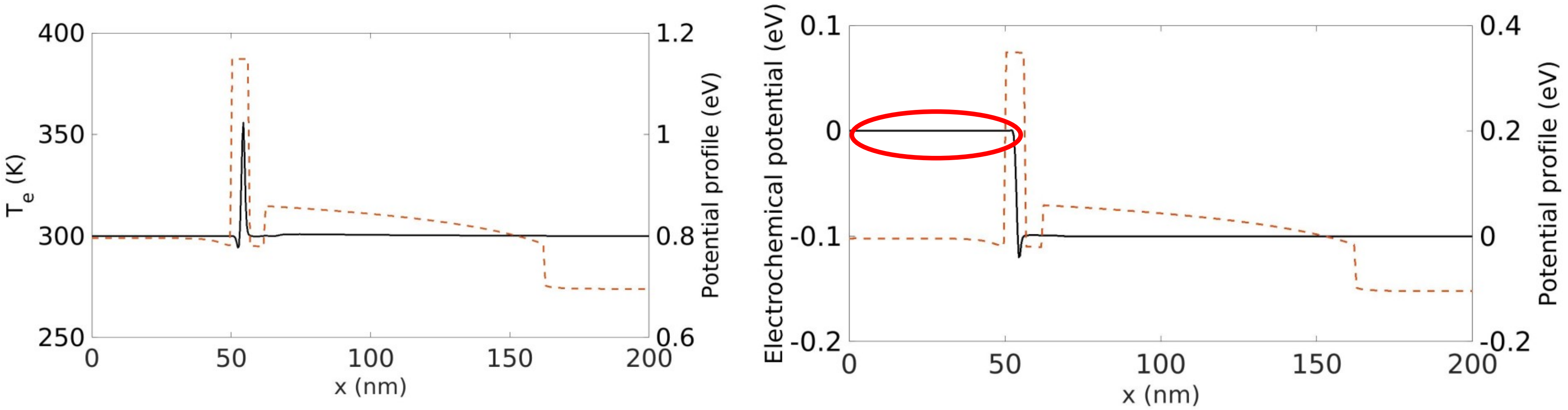
- ➢ Two current components in the access regions.
- ➢ At the barrier: phonon emission/absorption and back flow towards the contacts

Electron temperature and Chemical potential

ΔT=1 K, ΔV=0 V

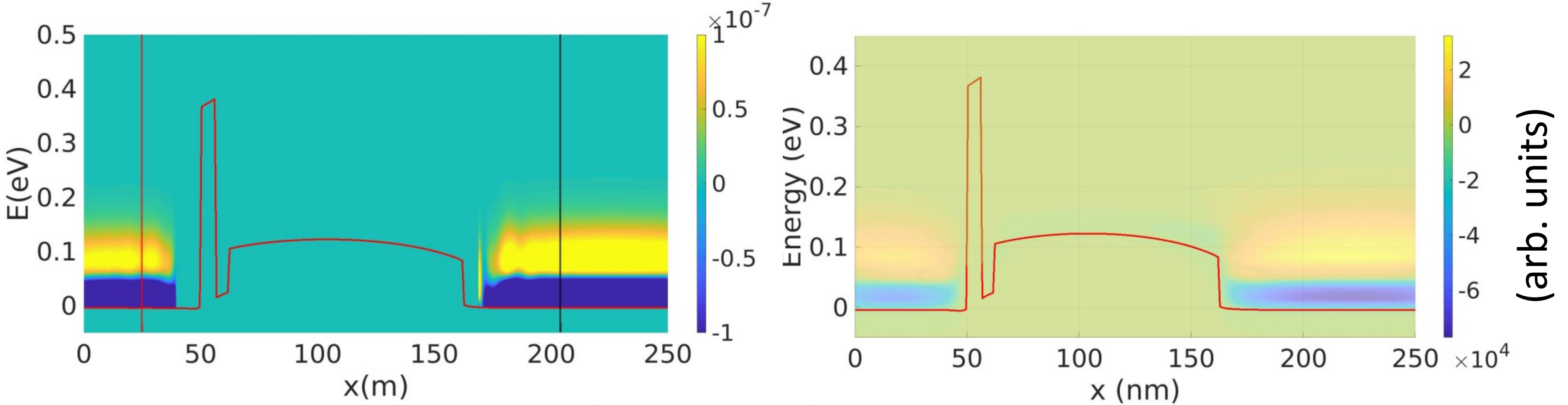


ΔT=0 K, ΔV=0.1 V



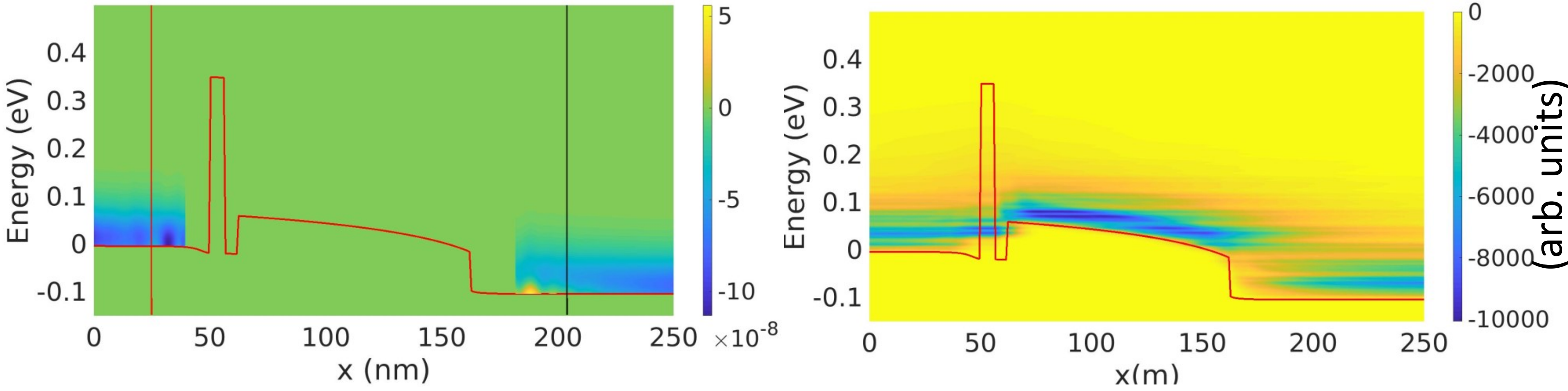
Difference of the Fermi-Dirac distributions

ΔT=1 K, ΔV=0 V


Δf_{FD}

Current spectrum

ΔT=0 K, ΔV=0.1 V

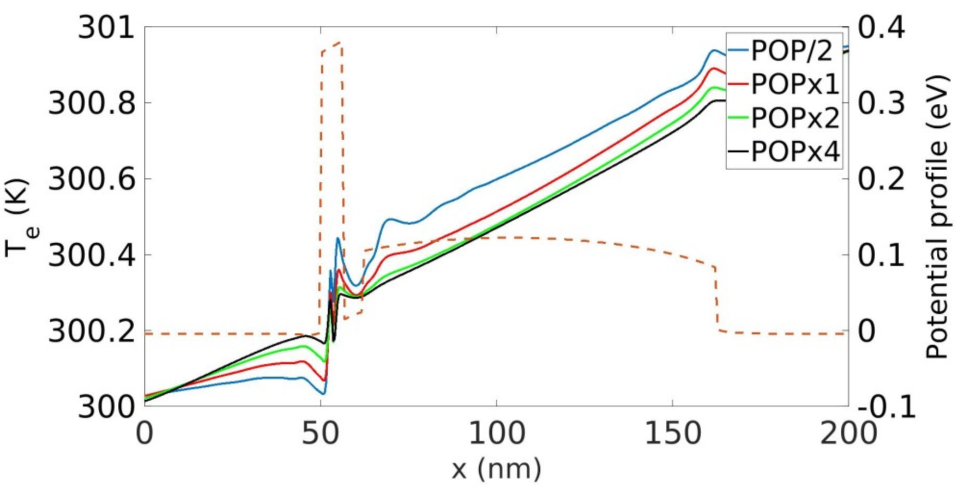


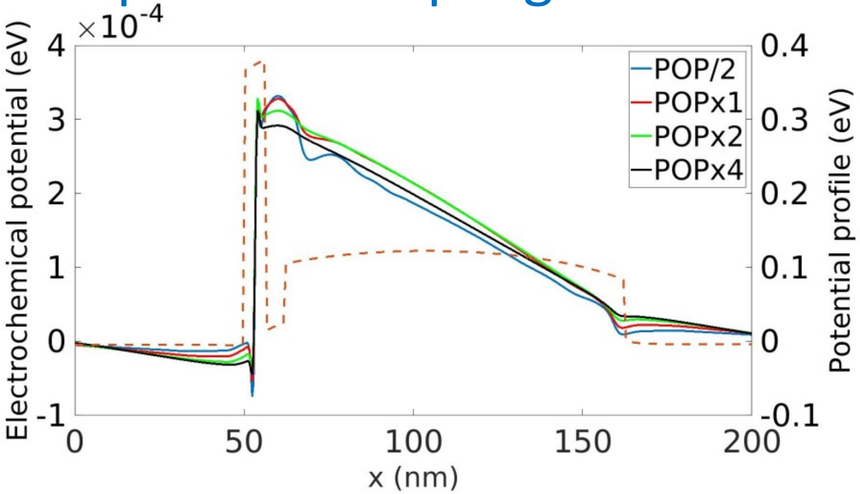
Origin of the reverse current component

- Reverse current: due to the variation of μ in the device.

- Increase of μ required to maintain the electron density with a ΔT_e.

Impact of the electron-phonon coupling





- Increasing coupling: T_e follow $T_{Lattice}$

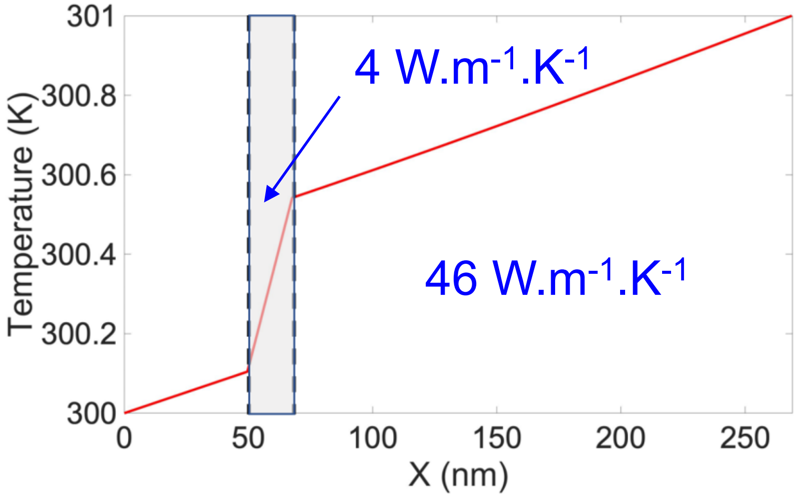
⇒ Larger T_e increase

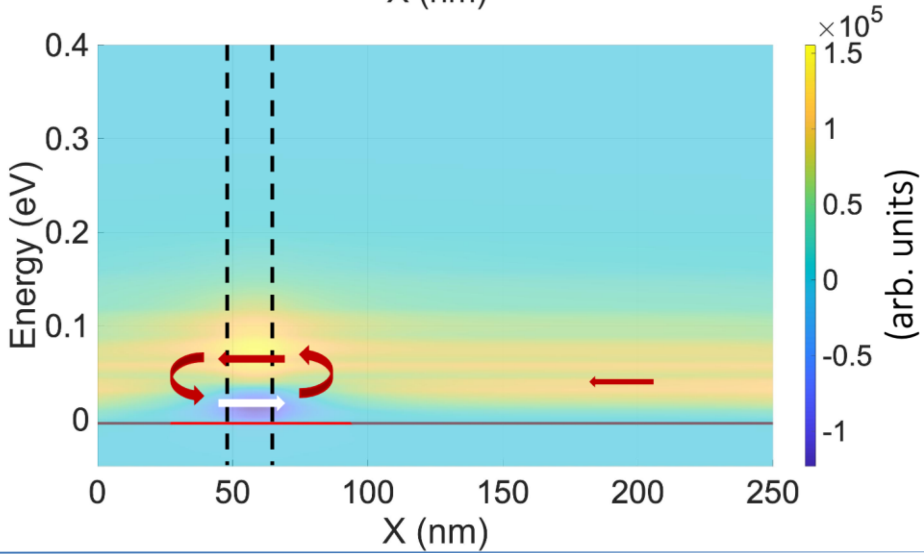
⇒ Larger μ decrease

Generalization of the Boomerang effect

- ➢ Boomerang/revolving effect obtained at any scattering center.

Variation of the thermal conductivity

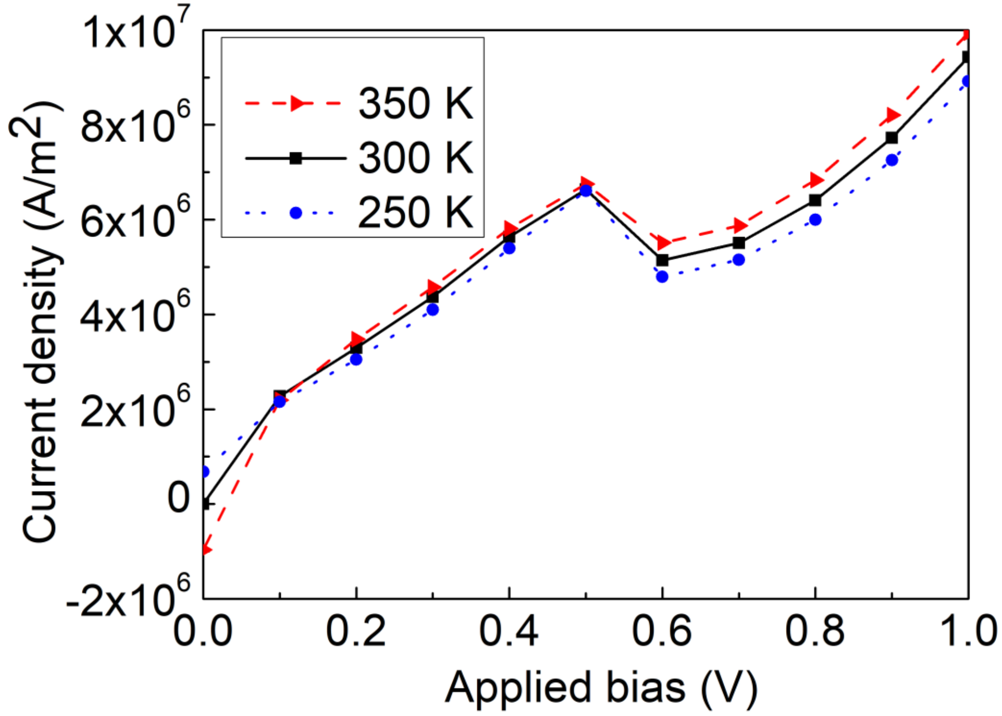




- ➢ Circular electron flux inside the region of low thermal conductivity

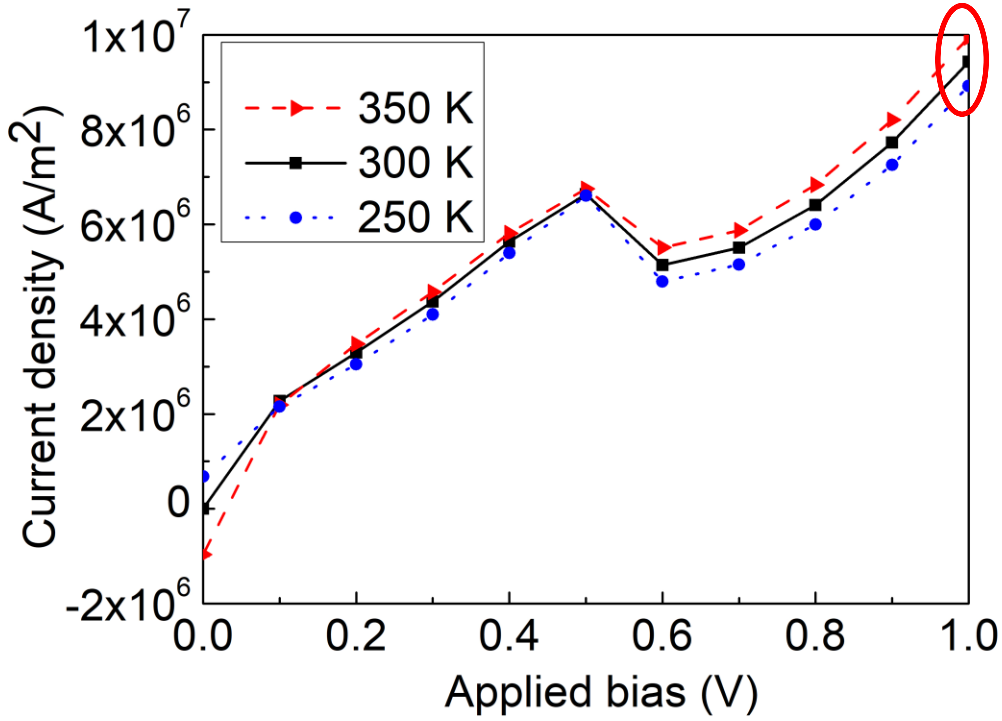
Experimental measurements

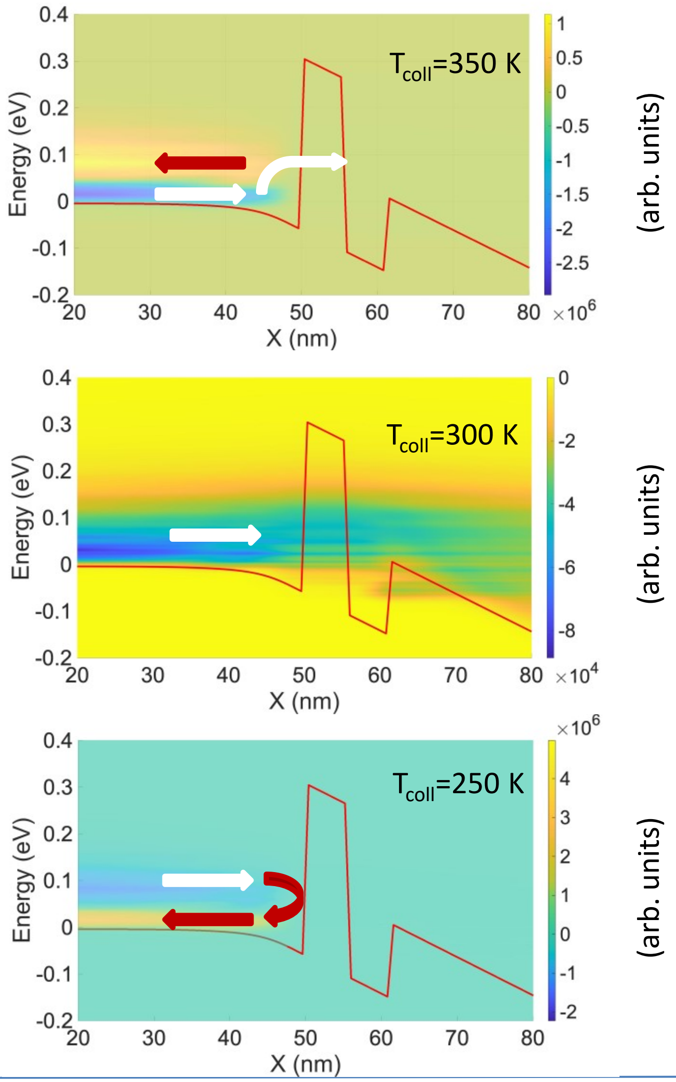
- I(V) at different temperature gradients:



Experimental measurements

- I(V) at different temperature gradients:





- Applying bias voltage, a temperature gradient in the opposite direction to the voltage (i.e. T_{Coll}=350K) induces an increase in the total current.

Conclusion

- Boomerang/revolving effect: control the direction flow of electrons in a given energy interval.

- Explained by non-equilibrium thermodynamic quantities (difference of the Fermi-Dirac distribution).

- Occurs at any type of scattering center (variation of the thermal conductivity).

- I(V) at different temperature gradients should be a straightforward approach to experimentally verify this effect.

Thank you!

NEGF for electrons

➢ Non-equilibrium Green's function with Poisson equation

- Retarded Green's function for a given transverse mode:

$$G^r_{k_t} = \left[(E-V)I - H_{k_t} - \underbrace{\Sigma^r_{L,k_t} - \Sigma^r_{R,k_t}}_{\text{Contacts}} - \underbrace{\Sigma^r_{S,k_t}}_{\text{Phonon scattering}}\right]^{-1}$$

Effective mass hamiltonian

- Lesser/Greater Green's functions:

$$G^{\lessgtr}_{k_t} = G^r_{k_t}\left(\Sigma^{\lessgtr}_{L,k_t} + \Sigma^{\lessgtr}_{R,k_t} + \Sigma^{\lessgtr}_{S,k_t}\right)G^{r\dagger}_{k_t}$$

- Acoustic phonon self-energy:

Deformation potential Acoustic phonon temperature

$$\Sigma^{\lessgtr}_{AC}(j,j,E) = \sum_{k'_t}\pi(2n_{k'_t}+1)\frac{\Xi^2 k_B T_{AC}(j)}{\rho u_s^2}G^{\lessgtr}_{k'_t}(j,j,E)$$

Mass density Sound velocity

- Polar optical phonon self-energy*:

$$\Sigma^{\lessgtr}_{\mathrm{POP},k_t}(j,j,E) = \frac{\lambda M^2}{2\pi S}\sum_{k'_t}\Big[(n_L(j)+1)G^{\lessgtr}_{k'_t}(j,j,E\pm\hbar\omega_L)$$
$$+(n_L(j))G^{\lessgtr}_{k'_t}(j,j,E\mp\hbar\omega_L)\Big]$$
$$\times\int_{\pi/L_t}^{\pi}\frac{\pi(2n_{k'_t}+1)}{\sqrt{(k_t-k'_t\cos\theta)^2+(k'_t\sin\theta)^2}}\mathrm{d}\theta$$

$$n_L(j) = (\mathrm{e}^{(\hbar\omega_L)/(k_B T_{\mathrm{POP}}(j))} - 1)^{-1}$$

$$M^2 = 2\pi\hbar\omega_L e^2\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)$$

θ is the angle between k_t and k'_t

$\lambda = 8$ Scaling factor – takes into account the diagonal approximation.

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* M. Moussavou *et al. Phys. Rev. Appl.* **10**, 064023 (2018).

NEGF for electrons

➢ Non-equilibrium Green's function

- Electron density:

$$n_j = -\mathrm{i}\int_{-\infty}^{+\infty} G^<(j,j;E)\mathrm{d}E \qquad \text{with } G^<(j,j;E) = \sum\nolimits_{k_t} \underbrace{(2n_{k_t}+1)}_{\text{Degeneracy of mode } k_t} G^<_{k_t}(j,j;E)$$

- Electron current density from position *j* to *j+1*:

$$\begin{aligned} J_{j\to j+1} &= \int_{-\infty}^{+\infty} \mathrm{d}E \frac{\mathrm{e}}{\hbar} \sum_{k_t} \frac{(2n_{k_t}+1)}{S} \left[H_{j,j+1} G^<_{k_t}(j+1,j;E) - G^<_{k_t}(j,j+1;E) H_{j+1,j}\right] \\ &= \int_{-\infty}^{+\infty} \mathcal{J}_{j\to j+1}(E)\mathrm{d}E \end{aligned}$$

- Electronic energy current: $J^E_{j\to j+1} = \int_{-\infty}^{+\infty} E\mathcal{J}_{j\to j+1}(E)\mathrm{d}E$

Self-consistent coupling with Poisson's equation

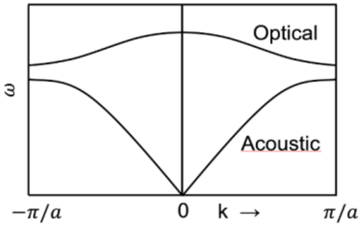
Heat equation

- Discretized heat equation:

$$\left[-\frac{\partial}{\partial x}\left[\kappa_{\text{th}}(x)\frac{\partial}{\partial x}T_{AC}(x)\right]\right]_j = Q_j$$

κ_{th} : thermal conductivity

T_{AC} : Acoustic phonon temperature (larger group velocity than POP)



- Q_j volumetric source term: power density (W.m^{-3}) exchanged between lattice and electrons

$$Q_j = -\nabla_j \cdot J^E \longleftarrow \text{Electronic energy current}$$

Q_j =0: no electron-POP coupling.
Q_j >0: power density transfer from lattice to electron --> heating.
Q_j <0: power density transfer from electron to lattice --> cooling.

- Polar optical phonons -->acoustic phonons -->thermal energy propagation
- Stationary conditions + Relaxation time approximation

$$\frac{(T_{\text{POP}}(j) - T_{AC}(j))C_{\text{POP}}}{\tau_{\text{POP}\to AC}} = Q_j$$

C_{POP} : thermal capacitance of the polar optical phonon (1.72 10^{6} J.(m^{3}.K)$^{-1}$)

$\tau_{\text{POP}\to AC}$: relaxation time POP-->AC (4.1610 10^{-12} s)

➡ T_{AC} and T_{POP} are injected in $\Sigma^{\lessgtr}_{AC}$ and $\Sigma^{\lessgtr}_{\text{POP}}$ of slide 10. (additionnal loop)

Electronic temperature: virtual probe technique

- Post-processing step: Green's function of the system already calculated
- Thermoelectric probe at the position *j*:

$$\Sigma^>(j;E) = -\mathrm{i}[1 - f_{\mathrm{FD}}(E,\mu_j,T_j^e)]LDOS(j;E)\nu_{\mathrm{coup}}$$

Fermi-Dirac distribution of e⁻ in the probe

$\mathrm{i}\frac{[G^>(j,j;E)-G^<(j,j;E)]}{2\pi}$

Probe/system coupling

$$\Sigma^<(j;E) = \mathrm{i}f_{\mathrm{FD}}(E,\mu_j,T_j^e)LDOS(j;E)\nu_{\mathrm{coup}}$$

- Simultaneous cancellation of the carrier and energy currents:

$$\begin{cases} \Delta J(j) = \int_{-\infty}^{+\infty} \Sigma^>(j;E)G^<(j,j;E)\mathrm{d}E - \int_{-\infty}^{+\infty} G^>(j,j;E)\Sigma^<(j;E)\mathrm{d}E = 0 \\ \Delta J^E(j) = \int_{-\infty}^{+\infty} E\Sigma^>(j;E)G^<(j,j;E)\mathrm{d}E - \int_{-\infty}^{+\infty} EG^>(j,j;E)\Sigma^<(j;E)\mathrm{d}E = 0 \end{cases}$$

(Newton-Raphson)

- Unique solution.

NEGF for phonon

- NEGF for electrons: Schrödinger equation

$$(E\mathbf{I}-\mathbf{H})\overline{\psi}=\bar{0} \quad \Longrightarrow \quad \left[G^{R}(E)\right]$$

- NEGF for phonons: dynamical equation

$$\omega^{2}\text{M}+\Phi_{nm}^{ij}\bar{R}=\bar{O} \qquad \text{with} \qquad \Phi_{nm}^{ij}=\frac{\partial^{2}V^{harm}}{\partial R_{n}^{i}\,\partial R_{m}^{j}}$$

Vibration frequency Mass of the atoms (matrix) 2nd order FC Displacement of the atoms

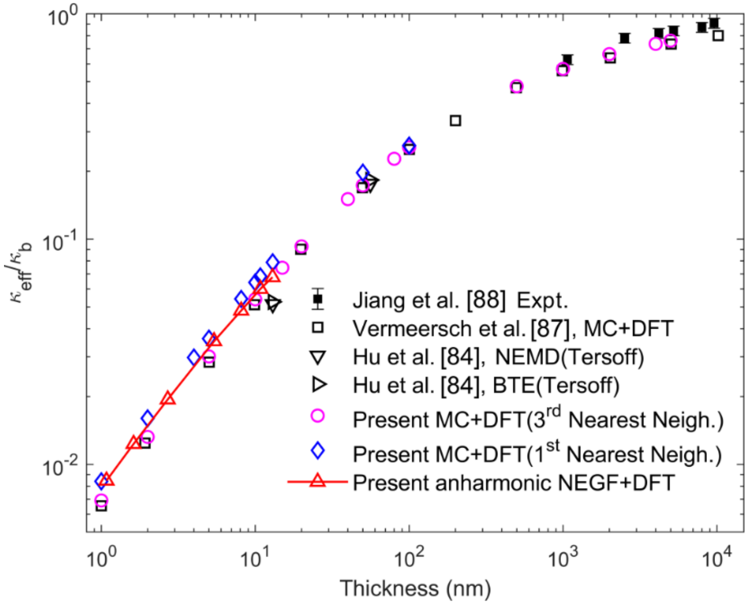
Retarded Green's function $$\mathbf{G}^{\mathrm{R}}(\omega)=[\omega^{2}\mathbf{I}-\mathbf{\Phi}-\mathbf{\Sigma}^{\mathrm{R}}(\omega)]^{-1}$$

- Anharmonic: N. Mingo, *Phys. Rev. B* **74**, 125402 (2006). (junctions)
J. S. Wang, N. Zeng, J. Wang, and C. K. Gan, *Phys. Rev. E* **75**, 061128 (2007).
M. Luisier, *Phys. Rev. B* **86**, 245407 (2012). (nanowires)
K. Miao *et al., Appl. Phys. Lett*. **108**, 113107 (2016). (Büttiker Probes)
J. H. Dai and Z. T. Tian, *Phys. Rev. B* **101**, 041301 (2020). (interfaces)
R. Rhyner and M. Luisier, *Phys. Rev. B* **89**, 235311 (2014). (NEGF coupling e-/ph!!)

NEGF for phonon

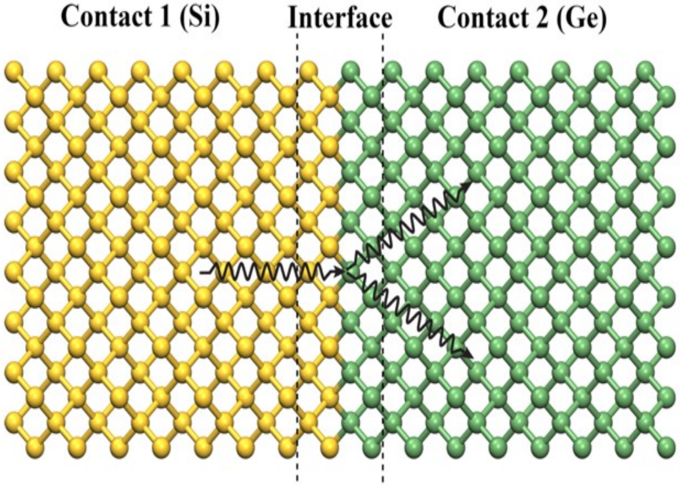
➢ Anharmonic phonon NEGF development: additional issues

Thermal conductivity Si film



Y. Guo, *et al., Phys. Rev. B*, **102**, 195412 (2020).

Si/Ge interface



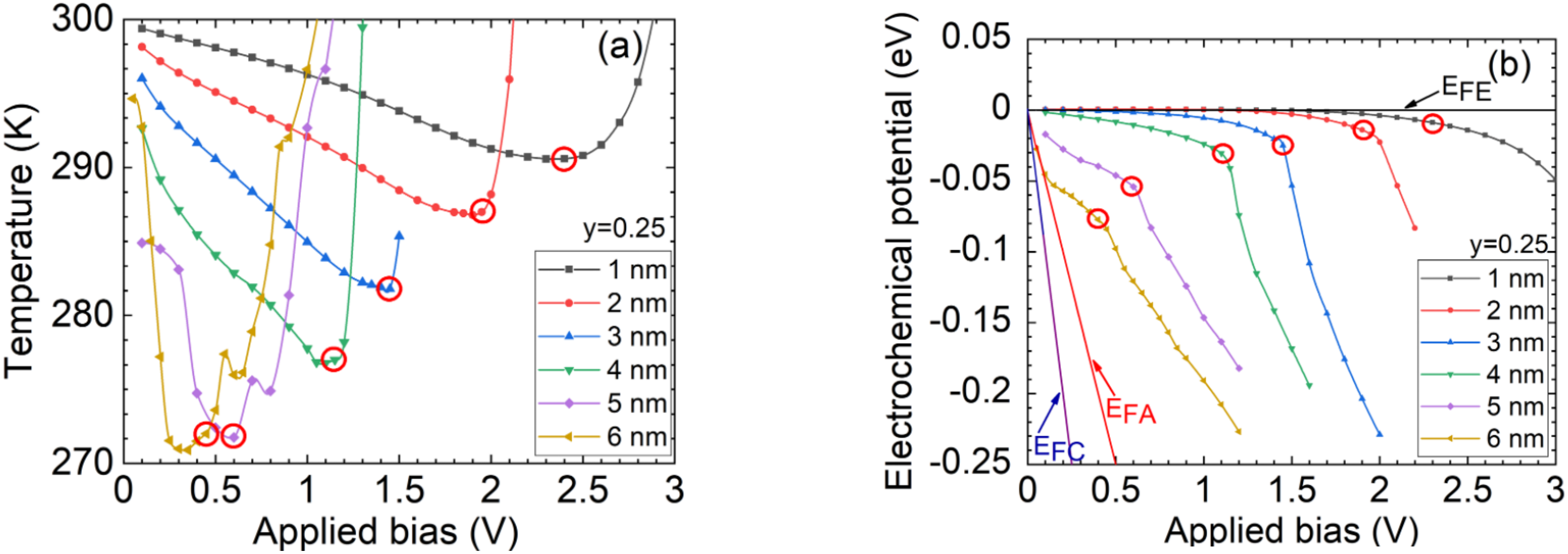
Y. Guo, *et al., Phys. Rev. B* **103** (17), 174306 (2021).

➢ Anharmonicity:

1) Non-local treatment of the phonon-phonon self-energies!
2) 4th order force constant might be needed…

→ NEGF for phonons can be only applied to rather small (tens of nanometers) systems.

Maximum electron cooling*



- ➢ Temperature minimum coincides very well with the resonance condition (highest current →best energy filtering).
- ➢ Temperature reduction increases with L_{Emit}.
- ➢ Electrochemical potential: best cooling when $R_{Emit} \approx R_{Coll}$.

*M. Bescond, *et al.*, *Phys. Rev. Appl.* **17,** 014001 (2022).

Electronic temperature: virtual probe technique

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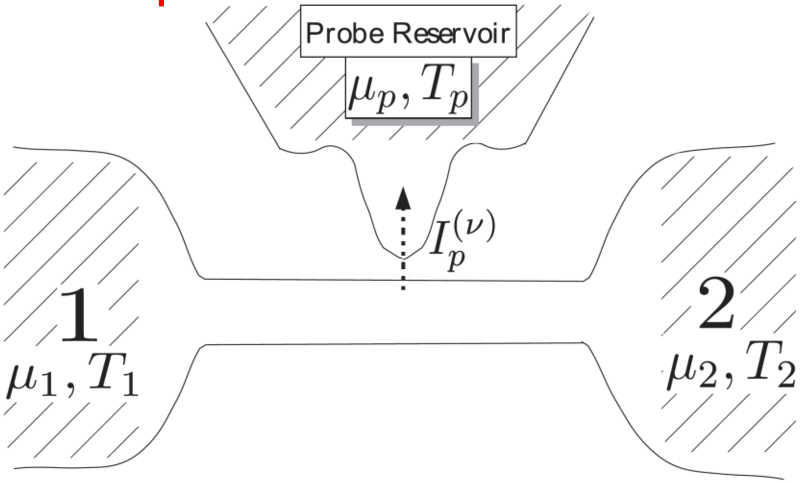

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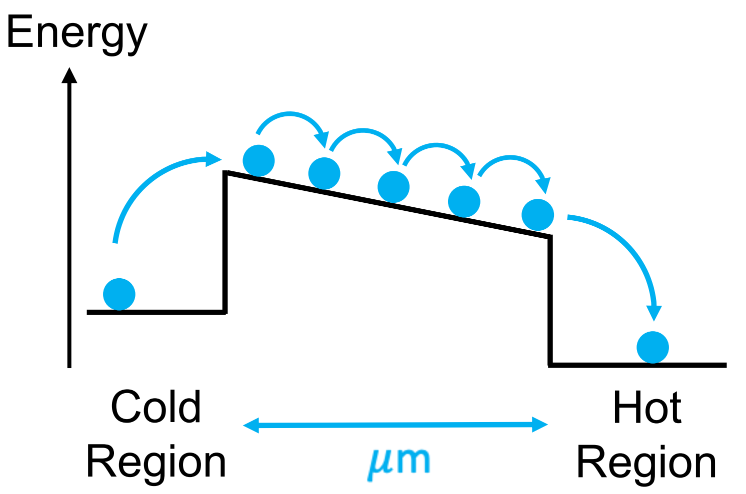
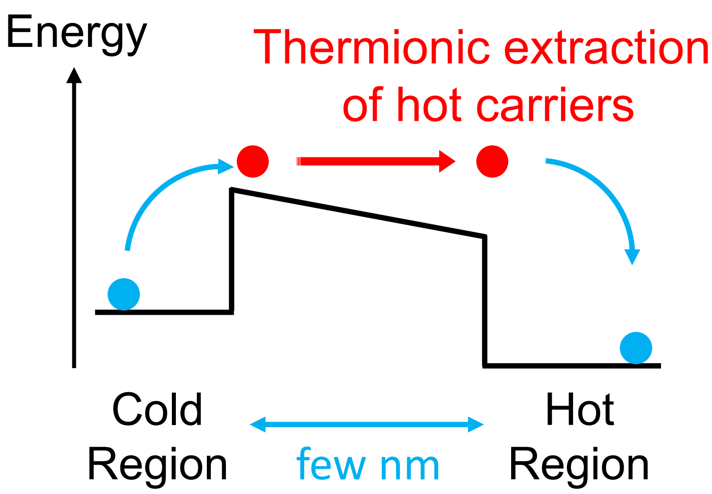
[1] C. A. Stafford, *Phys. Rev. B* **93**, 245403 (2016).

[2] A. Shastry and C. A. Stafford, *Phys. Rev. B* **94**, 155433 (2016).

Thermionic cooling*



Thermoelectric Peltier effect



Thermionic cooling

- ➢ Devices working in non-equilibrium regime.

Non-equilibrium ➜ Highest cooling power!

- ➢ Exploratory field: strong theoretical support.

Goal: use nano-structures to improve cooling efficiency.

*G. D. Mahan, *J. Appl. Phys.*, **76**, 4362 (1994).

*G. D. Mahan and L. M. Woods, *Phys. Rev. Lett.*, **80**, 4016 (1998).